

# Rocco Martinazzo

Università degli Studi di Milano

Homepage: <http://users.unimi.it/cdtg/rocco/home-rocco.shtml>

ResearcherID: B-5192-2011

Office: via Golgi 19  
20133, Milan, Italy

☎ +39 3496079713

✉ [rocco.martinazzo@unimi.it](mailto:rocco.martinazzo@unimi.it)



## Personal Information

Date of Birth	November 2, 1973
Place of Birth	Milan, (MI) Italy
Nationality	Italian
Marital Status	Married

## Education

- 2015-present **Associate Professor**, *Università degli Studi di Milano*, Milan, Italy.  
Dipartimento di Chimica
- 2012-2104 **Assistant Professor**, *Università degli Studi di Milano*, Milan, Italy.  
Dipartimento di Chimica
- 2004-2012 **Assistant Professor**, *Università degli Studi di Milano*, Milan, Italy.  
Dipartimento di Chimica-Fisica ed Elettrochimica
- 2002-2004 **PostDoc Fellow**, *Università degli Studi di Milano*, Milan, Italy.  
Project title: *Study of chemical reactions at catalytically relevant metal surfaces by means of first-principles methods and classical, quantum and mixed quantum-classical dynamical simulations* Supervisor: Prof. G. F. Tantardini
- 1999-2002 **Ph.D. in Chemical Sciences and Technologies**, *Università degli Studi di Milano*, Milan, Italy.  
Thesis title: *The  $\text{LiH}_2^+$  system: interaction forces and quantum dynamics* Supervisor: Prof. E. Gianinetti
- 1992-1998 **Master of Science in Chemistry**, *Università degli Studi di Milano*, Milan, Italy, GPA:110/110 *Cum Laude*.  
Thesis title: *Application of the Spin-Coupled Valence-Bond theory to the calculation of astrophysically relevant ion-molecule interaction potentials* Supervisor: Prof. M. Raimondi
- 1987-1992 **High School Diploma**, *ITIS Maria Curie*, Milano, Italy, GPA:60/60.  
Technical High School for Food Technologies

## Awards, Fundings and Scholarships

- 2018 **NEQRate**, *computational grant at CINECA HPC center (ca. 60,000 € worth).*
- 2017 **ExGas**, *Grant from Unimi, Development Plan for Athenaeum (7,400 € worth).*
- 2017 **ASN**, *National academic qualification as Full Professor in Physical Chemistry (03/A2).*
- 2016 **EuroPAH**, *PI of the local unit Unimi acting as Partner organization of the H2020-MSCA-ITN-2016 network (EU Grant n. 722346).*
- 2014 **LISA-MolrGr**, *computational grant at CINECA HPC center (80,000 € worth).*

- 2014 **ASN**, *National academic qualification as Associate Professor in Physical Chemistry (03/A2).*
- 2013 **LISA-IrGrappe**, *computational grant at CINECA HPC center (62,000 € worth).*
- 2013 **NEXT fellowship**, *Invited scientist fellowship to LCAR, Toulouse.*
- 2009-2011 **PRIN-2009C28YBF**, *member of the Milano research unit.*
- 2008 **Grant from the Università Franco-Italiane**, *support for the co-tutorship of a PhD project.*
- 2006-2008 **PRIN-2006030944**, *member of the Milano research unit.*
- 2004-2006 **PRIN-2004034838**, *member of the Milano research unit.*
- 2001-2002 **Max Planck Society**, *financial support to the visit at the Theoretical Chemistry group of prof. Franco Antonio Gianturco.*
- 1992-1998 **Scholarship**, *from Istituto per il diritto allo Studio Universitario.*
- 1992 **Silver medal**, *XXIVth International Chemistry Olympiads, Pittsburg, United States. July, 11-20*
- 1992 **Attestato di Benemerenzza**, *for merits from the Associazione Periti Industriali di Milano.*

## Experience

### Research

- 2015-present **Chemical Dynamics Theory Group**, *R. Martinazzo*, Università degli Studi di Milano, Milan, Italy.  
Principal Investigator
- 2013 **LCAR**, *D. Lemoine*, Université Paul Sabatier, Toulouse, France.  
Invited scientist
- 2002-2014 **Chemical Dynamics Theory Group**, *G.F. Tantardini*, Università degli Studi di Milano, Milan, Italy.  
Senior member
- Winter 2005-2006 **Theoretical Chemistry Group**, *P. Saalfrank*, Institute of Chemistry, University of Potsdam, Potsdam, Germany.  
Visiting scientist
- 2000-2002 **Theoretical Chemistry Group**, *F. A. Gianturco*, Università di Roma La Sapienza, Rome, Italy.  
Visiting student

### Academia

- March 2019 **EPoLM-4**, *4th Workshop on Energetic processing of large molecules*, Madrid, Spain, Invited Talk: "The interaction of H atoms with coronene: a quantum chemist's perspective".
- Sept 2018 **ETSF**, *23rd Workshop on electronic excitations: interdisciplinary views on quantum many-body theory*, Milano, Italy, Invited Talk: "Why Silicon is not Carbon?".
- Aug 2018 **ECOSS 34**, *34th European Conference on Surface Science*, Aarhus, Denmark, Program Committee.
- Jun 2017 **Challenges in reaction dynamics of gas-surface interactions**, *Methodological advances in dissipative and non-adiabatic process*, Albi, France, Co-organizer.
- Jul 2015 **13th International workshop on Quantum Reactive Scattering**, Salamanca, Spain, Invited Talk: "Quantum dynamics of hydrogen atoms on graphene".

- Oct 2014 **16th Workshop on Dynamical Phenomena at Surfaces**, Madrid, Spain, Invited Talk: "Adsorption, clustering and reactions of hydrogen atoms on graphene".
- May 2014 **Quantum and Classical Complexity: From Atoms to Biosystems**, Frankfurt, Germany, Invited Talk: "Effective mode representation of structured environments: towards *first principles* quantum dynamics of hydrogen atoms on graphene".
- Nov 2013 **Scattering of atoms and molecules from surfaces**, Potsdam, Germany, Invited Talk: "Hydrogen atoms on graphene: structure, energetics and dynamics".
- Apr 2013 **Exploring mechanisms for H<sub>2</sub> formation on very small carbonaceous grains and PAHs of astrophysical interest**, Toulouse, France, Invited Talk: "Adsorption and reaction of hydrogen atoms on graphitic substrates".
- Apr 2013 **Rome School on Open Systems and the Quantum-Classical Boundary**, Rome, Italy, Invited Talk: "Effective mode representation of structured environments".
- Sept 2012 **GraphEL**, Mykonos, Greece, Talk: "Spin-coupling around a carbon atom vacancy in graphene".
- Nov 2011 **Leiden Universiteit**, Leiden, The Netherlands, Van Marum Colloquium: "Effective mode representation of quantum mechanical energy transfer to surfaces".
- Sept 2011 **Meeting ARCHES- Adsorption, Reactivite et Controle de l'Hydrogene En interaction avec des Surfaces**, Alenya, Perpignan, France, Invited Talk: "Interaction of hydrogen atoms with carbon *sp*<sup>2</sup> structures".
- Sept 2011 **Challenges in modelling the reaction chemistry of interstellar dust**, Leiden, The Netherlands, Talk: "Interaction of hydrogen atoms with carbon *sp*<sup>2</sup> structures: adsorption energetics and Eley-Rideal dynamics".
- May 2011 **Theoretical Molecular Dynamics with Surfaces and PAHs**, Toulouse, France, Invited Talk: "Hydrogen formation on graphitic surfaces: energetics and dynamics of elementary processes".
- May 2011 **GraphITA**, Gran Sasso National Laboratories, Assergi, L'Aquila, Italy, Invited Talk: "The effect of atomic-scale effects on graphene electronic structure".
- Dec 2010 **Elementary Reactive Processes at Surfaces**, Bordeaux, France, Invited Talk: "Adsorption, clustering and reactions of H atoms on graphene".
- Sept 2010 **XXXIX congresso nazionale di chimica fisica**, *Organizing committee*, Stresa (VB), Italy.
- Sept 2010 **ECOSS 27, 27th European Conference on Surface Science**, Groningen, The Netherlands, Talk: "Symmetry-induced band-gap opening in graphene superlattices".
- Sept 2009 **ECOSS 26, 26th European Conference on Surface Science**, Parma, Italy, Chairman at the session: "Nanoelectronic materials and graphene".
- Dec 2008 **Winter modeling workshop**, Pisa, Italy, Invited Talk: "Wavepacket approaches to system-bath quantum dynamics".
- Sept 2008 **Multidimensional Quantum Mechanics with Trajectories**, *workshop organized by CCP6*, Leeds, United Kingdom, Invited Talk: "Local coherent-state approximation to system-bath quantum dynamics".
- Jul 2008 **ECOSS 25, 25 th European Conference on Surface Science**, Liverpool, United Kingdom, Invited Talk: "Theoretical study of hydrogen adsorption and dynamics on graphitic surfaces".
- Feb 2008 **XXXVII Congresso Nazionale di Chimica Fisica**, Camogli (GE), Italy, Talk: "The influence of quantum reection on the Eley-Rideal hydrogen formation reaction at interstellar cloud conditions".
- Aug 2007 **Elementary Reactive Processes at Surfaces**, *workshop organized by Donostia International Physics Center*, Donostia (S. Sebastian), Spain, Invited Talk: "Quantum studies of Hydrogen dynamics on graphite surfaces".

- Jul 2007 **Mathematical challenges in Quantum Chemistry Problems**, *interdisciplinary workshop at the Mathematics Institute of University of Warwick, Coventry, United Kingdom*, Invited Talk: "The Local Coherent-State Approach to System-Bath Quantum Dynamics and Its Extensions".
- June 2007 **The Quantum World in Real Time: Is it accessible?**, *workshop organized by the Weizmann Institute of Science, Safed, Israel*, Invited Talk: "The Local Coherent State Approach to System-Bath Quantum Dynamics".

### Teaching

- 2016-present **Physical Chemistry B - Solid state**, *Master Degree in Chemistry*, Lecturer.
- 2016 **Mathematical methods in chemistry**, *Master Degree in Chemistry*, Lecturer.
- 2015-present **Physical Chemistry III**, *Bachelor Degree in Chemistry*, Lecturer.
- 2009-2014 **Quantum Chemistry**, *Bachelor Degree in Chemistry*, Lecturer.
- 2011 **The role of phonons in Dynamics of molecule-surface reactions**, *Master Degree in Chemistry, Leiden, The Netherlands*, Invited lecturer.
- 2006-present **Theoretical Chemistry**, *Master Degree in Chemistry*, Lecturer.
- 2008-2010 **Quantum Chemistry**, *Bachelor Degree in Chemistry*, Lecturer.
- 2011,2007,2005 **Chemical Dynamics**, *a course for the Doctorate School in Chemical Sciences*, Lecturer.
- 2008-2010 **Physical Chemistry B (Solid State)**, *Master Degree in Chemistry*, Teaching assistant.
- 2004-2006 **Theoretical Chemistry**, *Master Degree in Chemistry*, Teaching assistant.

### Academic roles

- 2018-present Member of the scientific committee of the Department of Chemistry
- 2016-present Scientific Director of the Chemistry Library
- 2015-present Unimi referent for supercomputing at CINECA
- 2015-present Chemistry referent for admission tests at Unimi

### Languages

Italian **mother tongue**  
English **fluent**

### Computer skills

OS	Linux/Unix, Windows	programming	Fortran 77/90, Bash
job-related	Linux SA	typography	L <sup>A</sup> T <sub>E</sub> X, Microsoft Office

### Scientific Interests

- Graphene and related carbon-based materials
- Electronic structure and transport at the nanoscale
- Dissipative quantum dynamics and quantum transport
- Wavepacket methods for real-time quantum dynamics in large systems
- Dynamics in the gas-phase and at the gas-surface interface
- Interstellar Chemistry

## ISI Citation metrics<sup>†</sup>

H-index	23	Publications	71
Overall citations	1571	Average	23.45
† See <a href="http://www.researcherid.com/rid/B-5192-2011">http://www.researcherid.com/rid/B-5192-2011</a> for updates.			

## Google Scholar

H-index	26	Since 2014	17
Overall citations	2274	Since 2014	1286